

RN 22772-23-2 REGISTRY

CN Benzofuran, 2-(4-methylphenyl)-5-phenyl- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Benzofuran, 5-phenyl-2-p-tolyl- (8CI)

FS 3D CONCORD

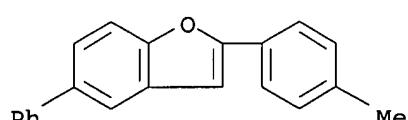
MF C21 H16 O

LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, IFICDB, IFIPAT, IFIUDB,
USPATFULL

(*File contains numerically searchable property data)

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C6	C6	6	C6	46.150.18	2
C4O-C6	OC4-C6	5-6	C8O	333.200.32	1



$R_{1a} = \text{phenyl}$

$R_{1b} = \text{H}$

$R_{2a} = R_{2b} = \text{Hydrogen}$

$R^{17} =$

Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	85923	pH 1	(1) ACD
Bioconc. Factor (BCF)	85923	pH 4	(1) ACD
Bioconc. Factor (BCF)	85923	pH 7	(1) ACD
Bioconc. Factor (BCF)	85923	pH 8	(1) ACD
Bioconc. Factor (BCF)	85923	pH 10	(1) ACD
Boiling Point (BP)	456.0 +/- 14.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	68.84 +/- 3.0 kJ/mol		(1) ACD
Flash Point (FP)	243.1 +/- 12.4 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	2		(1) ACD
H acceptors (HAC)	1		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	118417	pH 1	(1) ACD
Koc (KOC)	118417	pH 4	(1) ACD
Koc (KOC)	118417	pH 7	(1) ACD
Koc (KOC)	118417	pH 8	(1) ACD
Koc (KOC)	118417	pH 10	(1) ACD
logD (LOGD)	6.79	pH 1	(1) ACD
logD (LOGD)	6.79	pH 4	(1) ACD
logD (LOGD)	6.79	pH 7	(1) ACD
logD (LOGD)	6.79	pH 8	(1) ACD
logD (LOGD)	6.79	pH 10	(1) ACD
logP (LOGP)	6.795 +/- 0.360		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	284.35		(1) ACD
Vapor Pressure (VP)	4.54E-08 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.76 ((C) 1994-2003 ACD)

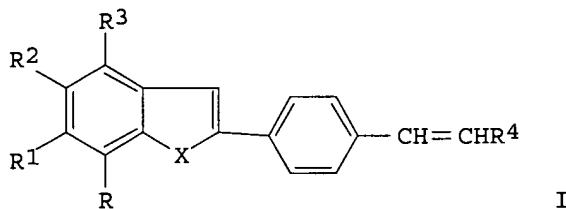
9 REFERENCES IN FILE CA (1907 TO DATE)
9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 86:56762 CA
TI Stilbene fluorescent whiteners and compositions brightened with them
IN Crounse, Nathan N.; Desai, Kantilal B.
PA Sterling Drug, Inc., USA
SO U.S., 10 pp. Division of U.S. 3,932,301.
CODEN: USXXAM
DT Patent
LA English
IC C07D209-04
NCL 260240000D
CC 40-11 (Dyes, Fluorescent Whitening Agents, and Photosensitizers)
FAN.CNT 4

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3993645	A	19761123	US 1975-573166	19750430
	US 3781279	A	19731225	US 1971-118076	19710223
	US 3932301	A	19760113	US 1973-364248	19730529
PRAI	US 1971-118076		19710223		
	US 1973-364248		19730529		

GI



AB Fluorescent whiteners [I, R = H, Cl; R1, R2R3 = benzo; R1 = H, MeO; R1R2, R2R3 = benzofuro; R2 = H, Cl, Ph; R3 = H; R4 = benzene, naphthalene, biphenyl, phenanthrene residue; X = O, S, NH, NMe] were prepd. and whitened polyester fibers from the melt. Thus, .omega.- (phenylthio) -p-methylacetophenone [36734-50-6] was heated in polyphosphoric acid to give 2- (p-tolyl)benzothiophene [25664-47-5] and condensation with PhCH:NPh [538-51-2] in DMF in the presence of KOCMe3 gave I (R = R1 = R2 = R3 = H, R4 = Ph, X = S) [25664-50-0]. The other 19 I were similarly prepd.
ST benzothienylethylene fluorescent brightener; benzofuranylethylene fluorescent brightener; indolylethylene fluorescent brightener; polyester fiber fluorescent brightener; stilbene heterocycle fluorescent brightener
IT Polyester fibers, uses and miscellaneous
RL: USES (Uses)
(fluorescent brighteners for, heterocyclic stilbene derivs. as)
IT Fluorescent brighteners
(heterocyclic stilbene derivs., for polyester fibers)
IT 36734-50-6 51357-99-4 51358-00-0 61548-21-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of)
IT 29347-55-5

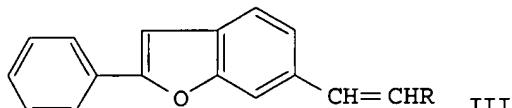
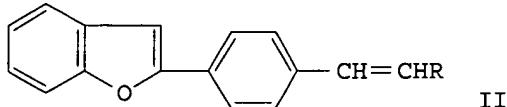
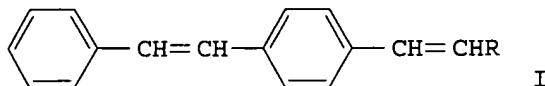
RL: USES (Uses)
 (fluorescent brightener, for polyester fibers, prepn. of)
 IT 51358-03-3P 51358-04-4P 51358-10-2P
 RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and cyclization of)
 IT 25664-50-0P 25664-53-3P 29335-23-7P 29335-29-3P 29344-58-9P
 29347-39-5P 29347-41-9P 29347-43-1P 29347-67-9P 29391-02-4P
 29399-40-4P 51357-97-2P 51357-98-3P 51358-02-2P 51358-06-6P
 51358-07-7P 51358-09-9P 51358-13-5P 58559-04-9P 58559-05-0P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and fluorescence spectrum of)
 IT 22772-22-1P 22950-16-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and reaction of, with benzalaniline)
 IT 25664-47-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and reaction with anil derivs.)
 IT 51358-11-3P 61548-22-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and reaction with benzalaniline)
 IT 22772-23-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and reaction with naphthalaniline)
 IT 22772-26-5P 51358-05-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and reaction with phenylbenzalaniline)
 IT 25664-48-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with arom. aldehyde derivs.)
 IT 51358-01-1
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with benzalaniline)
 IT 86-77-1 92-69-3 120-83-2
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with methylphenacyl chloride)
 IT 51358-08-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with phenylbenzalaniline)
 IT 4209-24-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with phenylphenol)
 IT 538-51-2 836-41-9 890-50-6 2362-79-0 18263-29-1 18263-30-4
 51357-73-4
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with tolyl deriv. of heterocyclic compd.)

REFERENCE 2

AN 85:48246 CA
 TI Anil synthesis. 11. Preparation of 4-styrylstilbene,
 4-(benso[b]furan-2-yl)stilbene, and .beta.- (2-phenylbenzo[b]furan-6-
 yl)styrene derivatives substituted in the 4'-position
 AU De Buman, Alain; Siegrist, Adolf E.
 CS Org.-Chem. Inst., Univ. Freiburg, Fribourg, Switz.
 SO Helvetica Chimica Acta (1974), 57(5), 1352-82
 CODEN: HCACAV; ISSN: 0018-019X
 DT Journal
 LA German

CC 40-11 (Dyes, Fluorescent Whitening Agents, and Photosensitizers)
Section cross-reference(s): 25, 27, 28

GI



AB Stilbene and styrene derivs. I-III (R = heterocyclic-substituted phenyl or phenylbenzofuranyl) (156), one of which is known as a fluorescent whitening agent, were prep'd. by the anil synthesis, i.e., by reaction of the 4-chloroanils of 4-stilbenecarboxaldehyde [40200-69-9], p-(2-benzofuranyl)benzaldehyde [53348-90-6], and 2-phenyl-6-benzofurancarboxaldehyde [53348-88-2] with heterocyclic-substituted toluenes or 2-aryl-6-methylbenzofurans in the presence of DMF and KOH or KOBu-tert. The absorption and fluorescence λ_{max} of the I-III are given. The anil synthesis produces a trans double bond exclusively, in contrast to the reaction of an aldehyde with a $(\text{EtO})_2\text{P}(\text{O})\text{CH}_2$ -substituted arom. compd., which gives a cis-trans mixt.

ST styrylstilbene whitener prepn spectra; benzofuranylstilbene whitener prepn spectra; phenylbenzofuranylstyrene whitener prepn spectra; stilbene deriv whitener; anil synthesis stilbene deriv

IT Molecular structure-property relationship
(fluorescence spectra, of styrylstilbenes and related compds.)

IT Fluorescence

Ultraviolet and visible spectra
(of benzofuranylstilbene, (phenylbenzofuranyl)styrene and styrylstilbene derivs.)

IT 33008-48-9

RL: RCT (Reactant)
(bromination or reaction of, with phenylbenzofurancarboxaldehyde chloroanil)

IT	25664-48-6P	53348-57-5P	53348-58-6P	53348-60-0P	53348-61-1P
	53348-62-2P	53348-63-3P	53348-64-4P	53348-65-5P	53348-66-6P
	53348-67-7P	53348-68-8P	53348-69-9P	53348-70-2P	53348-71-3P
	53348-72-4P	53348-73-5P	53348-74-6P	53348-75-7P	53348-76-8P
	53348-77-9P	53348-78-0P	53348-79-1P	53348-80-4P	53348-81-5P
	53348-82-6P	53348-83-7P	53348-84-8P	53349-04-5P	53349-05-6P
	53349-06-7P	53349-07-8P	53349-08-9P	53349-09-0P	53349-10-3P
	53349-11-4P	53349-12-5P	53349-13-6P	53349-14-7P	53349-15-8P
	53349-16-9P	53349-17-0P	53349-18-1P	53349-19-2P	53349-20-5P
	53349-21-6P	53349-22-7P	53349-23-8P	53349-24-9P	53349-25-0P
	53349-26-1P	53349-27-2P	53349-28-3P	53349-29-4P	53349-30-7P
	53349-31-8P	53349-32-9P	53349-33-0P	53349-34-1P	53349-35-2P
	53349-36-3P	53349-37-4P	53349-38-5P	53349-39-6P	53349-40-9P
	53349-41-0P	53349-42-1P	53349-43-2P	53349-44-3P	53349-45-4P
	53349-46-5P	53349-47-6P	53349-48-7P	53349-49-8P	53349-50-1P
	53349-51-2P	53349-52-3P	53349-53-4P	53349-54-5P	53349-55-6P
	53349-56-7P	53349-57-8P	53349-58-9P	53349-59-0P	53349-60-3P
	53349-61-4P	53349-62-5P	53349-63-6P	53349-64-7P	53349-65-8P

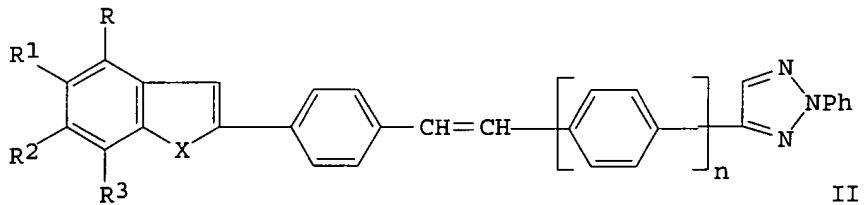
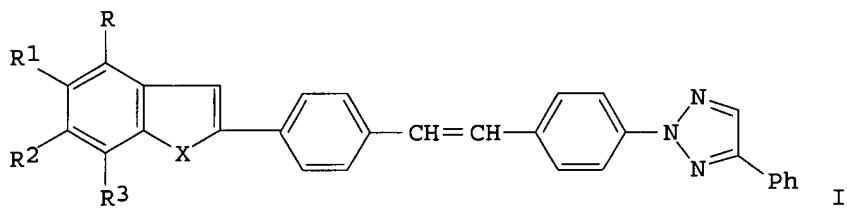
53349-66-9P	53349-67-0P	53349-68-1P	53349-69-2P	53349-70-5P
53349-71-6P	53349-72-7P	53349-73-8P	53349-74-9P	53349-75-0P
53349-76-1P	53349-77-2P	53349-78-3P	53349-79-4P	53349-80-7P
53349-81-8P	53349-82-9P	53349-83-0P	53349-84-1P	53349-85-2P
53349-86-3P	53349-87-4P	53349-88-5P	53349-89-6P	53349-90-9P
53349-91-0P	53349-92-1P	53349-93-2P	53349-94-3P	53349-95-4P
53349-96-5P	53349-97-6P	53349-98-7P	53349-99-8P	53350-00-8P
53350-01-9P	53350-02-0P	53350-03-1P	53350-04-2P	53350-05-3P
53350-06-4P	53350-07-5P	53350-08-6P	53350-09-7P	53350-10-0P
53350-11-1P	53350-12-2P	53350-13-3P	53350-14-4P	53350-15-5P
53350-16-6P	53350-17-7P	53350-18-8P	53350-19-9P	53350-20-2P
53350-21-3P	53350-22-4P	53402-88-3P	53402-89-4P	53415-36-4P
53415-37-5P	53415-38-6P	53415-39-7P	53415-40-0P	53415-41-1P
53415-42-2P	53829-78-0P			
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (prepn. and absorption and fluorescence spectra of)				
IT 53348-89-3P				
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and conversion to aldehyde)				
IT 53348-85-9P 53348-86-0P 53348-87-1P				
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and reaction of, with (methylphenyl)-substituted heterocyclic compds)				
IT 53348-88-2P 53348-90-6P				
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and reaction of, with chloroaniline)				
IT 59808-38-7P				
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and reaction of, with substituted benzaldehyde chloroanils)				
IT 6971-33-1				
RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with (aminophenyl)benzofuran)				
IT 780-21-2 3382-73-8 10480-32-7 17099-20-6 38607-96-4 38608-21-8				
RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with (benzofuranylphenyl)methylbenzotriazole)				
IT 4714-21-0 37163-68-1 52596-88-0 52823-30-0 58566-30-6 59808-39-8				
RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with [(chlorophenyl)imino]methylphenylbenzofuran)				
IT 599-69-9 640-57-3 835-71-2 1874-47-1 3287-02-3 3682-80-2				
16112-14-4 16112-16-6 16112-24-6 16151-04-5 16155-60-5				
16155-94-5 16155-95-6 16155-96-7 16156-01-7 16156-02-8				
16715-75-6 22720-98-5 22721-01-3 22772-23-2 22772-24-3				
22772-26-5 22772-28-7 22772-29-8 22772-30-1 22772-31-2				
22772-32-3 22950-16-9 24785-38-4 24785-40-8 25664-47-5				
31773-64-5 36843-34-2 36843-35-3 37421-68-4 37446-42-7				
37446-43-8 37582-50-6 38610-38-7 38610-40-1 42803-59-8				
52596-85-7 52596-86-8 52596-87-9 52823-29-7 52823-84-4				
52823-85-5				
RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with arom. aldehyde chloroanils)				
IT 106-47-8				
RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with arom. or heterocyclic aldehydes)				
IT 40200-69-9				
RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with chloroaniline)				
IT 782-18-3				
RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with nitronitrosotoluene)				

AN 84:181618 CA
 TI Styrene derivatives as fluorescent whiteners
 IN Kormany, Geza; Kabas, Guglielmo; Schlaepfer, Hans; Siegrist, Adolf E.
 PA Ciba-Geigy A.-G., Switz.
 SO Ger. Offen., 49 pp.
 CODEN: GWXXBX
 DT Patent
 LA German
 IC C07D; D06L
 CC 40-11 (Dyes, Fluorescent Whitening Agents, and Photosensitizers)
 Section cross-reference(s): 27, 28

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2535614	A1	19760304	DE 1975-2535614	19750809
	CH 598307	A	19780428	CH 1974-11109	19740814
	US 4014871	A	19770329	US 1975-601882	19750806
	US 4022772	A	19770510	US 1975-601883	19750806
	FR 2281932	A1	19760312	FR 1975-24947	19750811
	FR 2281932	B1	19790615		
	FR 2281934	A1	19760312	FR 1975-24946	19750811
	GB 1477958	A	19770629	GB 1975-33777	19750813
	GB 1477957	A	19770629	GB 1975-33773	19750813
	JP 51059926	A2	19760525	JP 1975-98162	19750814
	JP 51059945	A2	19760525	JP 1975-98161	19750814
	CH 619093	A3	19800915	CH 1977-8337	19770706
	CH 619093	B	19810313		
PRAI	CH 1974-11109		19740814		

GI



AB Styryl compds. I and II, where R, R2, and R3 = H or Me, R1 = H, Cl, Me, Ph, PhCH2, cyclohexyl, or MeO, X = O or S, and n = 0 or 1, are light-stable fluorescent whiteners for polyester fibers. These compds. were prep'd. by reaction of 2-(p-tolyl)benzofurans or -benzothiophenes with chloroanilins of p-(phenyl-1,2,3-triazolyl)benzaldehydes or 4-formyl-2-phenyl-1,2,3-triazole at 20-30.degree. in DMF in the presence of KOCMe3 or KOH, optionally while irradiating with uv light. Trypical of 28 fluorescent whiteners prep'd. are I (R = R2 = R3 = H, R1 = Ph, X = O) [59151-66-5], II (R-R3 = H, X = O, n = 1) [59151-67-6], and II (R-R3 = H, X = O, n = 0) [59151-68-7].

ST styryl fluorescent whitener; benzoxazole deriv fluorescent whitener; benzothiophene deriv fluorescent whitener; stilbene deriv fluorescent whitener; triazole deriv fluorescent whitener; polyester fiber fluorescent

whitener

IT Fluorescent brighteners
(benzoxazolyl- and benzothiophienyl(phenyltriazolyl)stilbenes,
polyester fibers)

IT Polyester fibers

RL: USES (Uses)
(fluorescent brighteners for, benzoxazolyl- and
benzothiophienyl(phenyltriazolyl)stilbenes as)

IT 59151-40-5 59151-41-6 59151-42-7 59151-43-8 59151-44-9
59151-45-0 59151-46-1 59151-47-2 59151-48-3 59151-49-4
59151-50-7 59151-51-8 59151-52-9 59151-53-0 59151-54-1
59151-55-2 59151-56-3 59151-57-4 59151-58-5 59151-59-6
59151-60-9 59151-61-0 59151-62-1 59151-63-2 59151-64-3
59151-65-4 59151-66-5 59151-67-6 59151-68-7

RL: USES (Uses)
(fluorescent brightener, for polyester fibers, prep. of)

IT 6206-78-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with (methylphenyl)benzofuran)

IT 59098-86-1 59099-28-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with (methylphenyl)benzofurans and -benzothiophenes)

IT 22720-98-5 22721-01-3 22772-23-2 22772-24-3 22772-26-5
22772-28-7 22772-29-8 22772-30-1 22772-31-2 22772-32-3
22772-33-4 25664-47-5 25664-48-6 58566-38-4

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with (phenyltriazolyl)benzaldehyde chloroanil)

REFERENCE 4

AN 84:123423 CA
TI Stilbene fluorescent whiteners and compositions whitened with them
IN Crounse, Nathan N.; Desai, Kantilal B.
PA Sterling Drug, Inc., USA
SO U.S., 10 pp. Continuation-in-part of U.S. 3,781,279.
CODEN: USXXAM

DT Patent

LA English

IC D06L

NCL 252301200W

CC 40-11 (Dyes, Fluorescent Whitening Agents, and Photosensitizers)

FAN.CNT 4

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3932301	A	19760113	US 1973-364248	19730529
	US 3781279	A	19731225	US 1971-118076	19710223
	US 3993645	A	19761123	US 1975-573166	19750430

PRAI US 1971-118076 19710223
US 1973-364248 19730529

GI For diagram(s), see printed CA Issue.

AB Fluorescent whiteners [I, R = H; (RR1), (R1R2) = benzo; R1 = H, Cl, Ph; R2 = H, MeO; R3 = H, Cl; R4 = Ph, substituted phenyl, naphthyl, phenanthrenyl; X = O, S, NH] and related dibenzofuran derivs. were prep'd. and used to whiten polyesters. Thus, 4-MeC₆H₄COCH₂SPh [36734-50-6] was heated with polyphosphoric acid at 180-90.degree. for 3 hr to give 2-p-tolylbenzothiophene [25664-47-5] which was condensed with PhCH:NPh [538-51-2] in DMF in the presence of KOCMe₃ to give I(R = R1 = R2 = R3 = H, R4 = Ph, X = S) [25664-50-0], excitation max. 359 nm, emission max. 412 nm. The other I were similarly prep'd.

ST fluorescent brightener stilbene; polyester fluorescent whitener; benzofuran fluorescent whitener; benzothiophene fluorescent whitener; indole fluorescent whitener

IT Fluorescent brighteners
([(arylviny)phenyl]benzofuran derivs., polyesters)

IT Polyesters, uses and miscellaneous
 RL: USES (Uses)
 (fluorescent brighteners for, [(arylvinyl)phenyl]benzofuran derivs. as)

IT 36734-50-6 37564-72-0 51357-99-4 51358-00-0
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (cyclization of)

IT 51358-03-3P 51358-04-4P 51358-10-2P
 RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and cyclization of)

IT 25664-50-0P 25664-53-3P 29335-23-7P 29335-29-3P 29344-58-9P
 29347-39-5P 29347-41-9P 29347-43-1P 29347-55-5P 29347-67-9P
 29391-02-4P 29399-40-4P 51357-97-2P 51357-98-3P 51358-02-2P
 51358-06-6P 51358-07-7P 51358-09-9P 51358-13-5P 58559-04-9P
 58559-05-0P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and fluorescence spectrum of)

IT 22772-26-5P 25664-47-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and reaction with arom. aldehyde anils)

IT 22772-23-2P 22950-16-9P 51358-05-5P 51358-11-3P 58559-03-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and reaction with benzaldehyde derivs.)

IT 25664-48-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with arom. aldehyde anils)

IT 51358-08-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with benzaldehyde deriv.)

IT 22772-22-1 51358-01-1
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with benzaldehyde derivs.)

IT 86-77-1 92-69-3 120-83-2
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with methylphenacyl chloride)

IT 4209-24-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with phenylphenol)

IT 890-50-6 2362-79-0 18263-29-1 18263-30-4 51357-73-4
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with tolylbenzofuran)

IT 538-51-2 836-41-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with tolylbenzothiophene)

REFERENCE 5

AN 82:113167 CA
 TI Anil synthesis. 10. Preparation of styryl derivatives of dibenzofurans
 AU Garmatter, Jacques; Siegrist, Adolf E.
 CS Org. Chem. Inst., Univ. Freibourg, Freibourg, Switz.
 SO Helvetica Chimica Acta (1974), 57(4), 945-79
 CODEN: HCACAV; ISSN: 0018-019X
 DT Journal
 LA German
 CC 40-11 (Dyes, Fluorescent Whitenning Agents, and Photosensitizers)
 GI For diagram(s), see printed CA Issue.
 AB Schiff bases of 2- and 3-dibenzofurancarboxaldehydes with p-ClC₆H₄NH₂ were
 condensed with p-tolyl substituted heterocyclic and carbocyclic arom.
 compds. in DMF in the presence of KOH or KOC(Me)₃ to give the
 corresponding styryl derivs. or styryl analogs (I, R = heterocyclic
 residue, arom. carbocyclic residue). The position of the absorption and

fluorescence max. of 3-dibenzofuran styryl derivs. was compared to the p-biphenyl residue-contg. derivs.

ST dibenzofuran styryl deriv; anil synthesis; fluorescent whiteners

dibenzofuryl styryl derivs

IT Fluorescent brighteners
(styryl dibenzofuran derivs.)

IT	52821-78-0	52821-79-1	52821-80-4	52821-81-5	52821-82-6
	52821-83-7	52821-84-8	52821-85-9	52821-86-0	52821-87-1
	52821-88-2	52821-89-3	52821-90-6	52821-91-7	52821-92-8
	52821-93-9	52821-94-0	52821-95-1	52821-96-2	52821-97-3
	52821-98-4	52821-99-5	52822-00-1	52822-01-2	52822-02-3
	52822-03-4	52822-04-5	52822-05-6	52822-06-7	52822-07-8
	52822-08-9	52822-09-0	52822-10-3	52822-11-4	52822-12-5
	52822-13-6	52822-14-7	52822-15-8	52822-16-9	52822-17-0
	52822-18-1	52822-19-2	52822-20-5	52822-21-6	52822-22-7
	52822-23-8	52822-24-9	52822-25-0	52822-26-1	52822-27-2
	52822-28-3	52822-29-4	52822-30-7	52822-31-8	52822-32-9
	52822-33-0	52822-34-1	52822-35-2	52822-36-3	52822-37-4
	52822-38-5	52822-39-6	52822-40-9	52822-41-0	52822-42-1
	52822-43-2	52822-44-3	52822-45-4	52822-46-5	52822-47-6
	52822-48-7	52822-49-8	52822-50-1	52822-51-2	52822-52-3
	52822-53-4	52822-54-5	52822-55-6	52822-56-7	52822-57-8
	52822-58-9	52822-59-0	52822-60-3	52822-61-4	52822-62-5
	52822-63-6	52822-64-7	52822-65-8	52822-66-9	52822-67-0
	52822-68-1	52822-69-2	52822-70-5	52822-71-6	52822-72-7
	52822-73-8	52822-74-9	52822-75-0	52822-76-1	52822-78-3
	52822-79-4	52822-80-7	52822-81-8	52822-82-9	52822-83-0
	52822-84-1	52822-85-2	52822-86-3	52822-87-4	52822-88-5
	52822-89-6	52822-90-9	52822-91-0	52822-92-1	52822-93-2
	52822-94-3	52822-95-4	52822-96-5	52822-97-6	52822-98-7
	52822-99-8	52823-00-4	52823-01-5	52823-02-6	52823-03-7
	52823-04-8	52823-10-6	52823-11-7	52823-12-8	52823-13-9
	52823-14-0	52823-15-1	52823-16-2	52823-17-3	52823-18-4
	52823-19-5	52823-20-8	52823-21-9	52823-22-0	52823-23-1
	52823-24-2	52823-25-3	52823-26-4	52823-27-5	52823-28-6
	52823-31-1	52823-32-2	52823-33-3	52823-34-4	52823-35-5
	52823-36-6	52823-38-8	52823-39-9	52823-40-2	52823-41-3
	52823-42-4	52823-43-5	52823-44-6	52823-45-7	52823-46-8
	52823-47-9	52823-48-0	52823-49-1	52823-50-4	52823-51-5
	52823-52-6	52823-53-7	52823-54-8	52823-55-9	52823-56-0
	52823-57-1	52823-58-2	52823-59-3	52823-60-6	52823-61-7
	52823-62-8	52823-63-9	52823-64-0	52823-65-1	52823-66-2
	52823-67-3	52823-68-4	52823-69-5	52823-70-8	52823-71-9
	52823-88-8	52871-56-4			

RL: PRP (Properties)
(fluorescent spectrum of)

IT 132-64-9

RL: RCT (Reactant); RACT (Reactant or reagent)
(nitration of)

IT	4106-66-5P	5410-97-9P	16155-56-9P	29021-90-7P	29021-91-8P
	42999-98-4P	52822-77-2P	52823-06-0P	52823-07-1P	52823-08-2P
	52823-72-0P	52823-73-1P	52823-74-2P	52823-75-3P	52823-76-4P
	52823-77-5P	52823-78-6P	52823-79-7P	52823-80-0P	52823-81-1P
	52823-82-2P	52823-83-3P	52823-84-4P	52823-85-5P	52823-86-6P
	52823-87-7P				

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT 32978-85-1 42999-98-4

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with (methylbenzotriazolyl)dibenzofuran)

IT	13533-31-8	15485-34-4	24588-83-8	38607-98-6	38607-99-7
	38608-00-3	38608-01-4	38608-18-3	38608-19-4	38608-20-7
	41855-64-5	51209-71-3			

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with (methylstyryl)dibenzofuran)

IT 10480-32-7 15485-22-0 17099-20-6 38607-92-0 38607-96-4
 38608-21-8 38608-23-0
 RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with (tolyloxadiazolyl)dibenzofuran)

IT 52823-06-0 52823-07-1 52823-08-2
 RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with [(chlorophenyl)imino]methyl]benzene)

IT 640-57-3 835-71-2 1874-47-1 2491-91-0 3287-02-3 3682-80-2
 4714-21-0 5998-46-9 10127-84-1 14770-90-2 16112-14-4 16112-16-6
 16112-22-4 16112-24-6 16112-26-8 16112-27-9 16112-32-6
 16151-04-5 16151-05-6 16155-57-0 16155-60-5 16155-94-5
 16155-95-6 16155-96-7 16156-01-7 16156-02-8 16715-75-6
 17453-11-1 17473-15-3 22720-97-4 22720-98-5 22721-01-3
 22772-23-2 22772-24-3 22772-26-5 22772-29-8 22772-30-1
 22772-31-2 22772-32-3 22950-16-9 24785-40-8 25664-47-5
 25664-48-6 31773-64-5 33008-48-9 36843-34-2 36843-35-3
 36843-36-4 37421-68-4 37446-37-0 37446-38-1 37446-41-6
 37446-42-7 37446-43-8 37446-44-9 37446-45-0 37446-47-2
 37446-48-3 37446-49-4 37506-95-9 37582-50-6 37582-51-7
 38610-35-4 38610-38-7 38610-40-1 38610-41-2 38610-43-4
 38610-44-5 38610-46-7 38610-47-8 38610-48-9 38610-49-0
 38610-50-3 38610-51-4 38610-52-5 38610-55-8 38662-76-9
 42196-66-7 42196-67-8 42196-68-9 42196-69-0 42803-59-8
 42944-39-8 52596-76-6 52596-77-7 52596-79-9 52596-80-2
 52596-81-3 52596-82-4 52596-83-5 52596-84-6 52596-86-8
 52596-87-9 52596-88-0 52596-89-1 52596-90-4 52596-93-7
 52596-94-8 52596-95-9 52823-09-3 52823-29-7 52823-30-0
 RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with [(chlorophenyl)imino]methyl]dibenzofuran)

IT 5397-82-0
 RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with chloroaniline)

IT 106-47-8 3762-25-2
 RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with dibenzofurancarboxaldehyde)

REFERENCE 6

AN 81:27212 CA
 TI Benzofurans, benzothiophenes, and naphthofurans as fluorescent whiteners
 IN Crounse, Nathan N.; Desai, Kantilal B.
 PA Sterling Drug Inc.
 SO Fr. Demande, 23 pp.
 CODEN: FRXXBL
 DT Patent
 LA French
 IC C09K; C08K; D06L
 CC 40-11 (Dyes, Fluorescent Whitening Agents, and Photosensitizers)
 FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	FR 2171128	A1	19730921	FR 1973-3777	19730202
	FR 2171128	B1	19770902		
	US 3833510	A	19740903	US 1972-224296	19720207
	CA 988927	A1	19760511	CA 1973-161971	19730124
	IT 977194	A	19740910	IT 1973-48053	19730205
	GB 1382544	A	19750205	GB 1973-5635	19730205
	JP 48091128	A2	19731127	JP 1973-14851	19730207

PRAI US 1972-224296 19720207
 AB Fluorescent whiteners [I, R = H, Me, MeO, Ph, Cl, F, CN; (RR1) = benzo; R1 = H, Cl; R2 = H, Me, HOCH₂CH₂; X = O, S] were prep'd. and were esp. useful for whitening polyester fibers by melt incorporation. Thus, a mixt. of 2-p-tolylbenzothiophene and p-HO₂CC₆H₄CH:NPh was heated in DMF in the

presence of KOCMe₃ to give fluorescent whitener (I, R = R₁ = R₂ = H; X = S) [50618-24-1].

ST benzofuran fluorescent whitener; benzothiophene fluorescent whitener; naphthofuran fluorescent whitener; stilbene fluorescent whitener; carboxystilbene fluorescent whitener

IT Fluorescent brighteners
 ([(carboxyphenyl)vinyl]phenyl]benzofuran analogs and derivs.,
 polyester fibers)

IT Polyester fibers
 RL: USES (Uses)
 (fluorescent brighteners for, [(carboxyphenyl)vinyl]phenyl]benzofuran
 analogs and derivs. as)

IT 50325-20-7P 50370-39-3P 50618-24-1P 50618-25-2P 50618-26-3P
 50618-27-4P 50618-28-5P 50618-29-6P 50618-30-9P 50618-31-0P
 50618-33-2P 50618-34-3P 50618-35-4P 50618-36-5P 50618-37-6P
 50618-38-7P 50618-39-8P 50618-40-1P 51331-97-6P
 RL: IMF (Industrial manufacture); PREP (Preparation)
 (prepn. of)

IT 22772-22-1 22950-16-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with anilinophthalide)

IT 33125-69-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with chlorotolylbenzofuran)

IT 4209-24-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with dichlorophenol)

IT 95-77-2 371-41-5
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with methylphenacyl chloride)

IT 3939-34-2
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with p-tolylbenzothiophene in presence of potassium
 tert-butyrate)

IT 25664-47-5
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with terephthalaldehydic acid anil in presence of
 potassium tert-butyrate)

IT 22772-23-2 22772-24-3 22772-26-5
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with terephthalaldehydic acid anil)

IT 25664-48-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with terephthalaldehydic acid anil in the presence of
 potassium tert-butyrate)

IT 51331-98-7
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with terephthalidic acid anil in the presence of
 potassium tert-butyrate)

REFERENCE 7

AN 80:134944 CA
 TI Stilbene fluorescent whiteners
 IN Crounse, Nathan N.; Desai, Kantilal B.
 PA Sterling Drug Inc.
 SO U.S., 7 pp.
 CODEN: USXXAM
 DT Patent
 LA English
 IC C09B
 NCL 260240000CA
 CC 40-11 (Dyes, Fluorescent Whitening Agents, and Photosensitizers)
 FAN.CNT 4

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3781279	A	19731225	US 1971-118076	19710223
	US 3932301	A	19760113	US 1973-364248	19730529
	US 4111962	A	19780905	US 1973-398673	19730919
	US 3993645	A	19761123	US 1975-573166	19750430
PRAI	US 1971-118076	19710223			
	US 1973-364248	19730529			
AB	Fluorescent whitener [I, R = H, (RR1) = benzo; R1 = H, Cl, Ph; R2 = H, Me, Cl; (R2R3) = benzo; R3 = H, Cl; R4 = Ph and substituted Ph, C10H7, phenanthrenyl, biphenyllyl; X = O, S, NH] were prep'd. and were melt incorporated into polyesters to give shades of whiteness in the pink and blue range. Thus, 2-(p-tolyl)benzothiophene was treated with p-MeOC ₆ H ₄ CH:NHPh in the presence of KOCMe ₃ to give fluorescent whitener I (X = S, R = R1 = R2 = R3 = H, R4 = p-MeOC ₆ H ₄) [29344-58-9]. The other I were similarly prep'd.				
ST	stilbene fluorescent whitener; polyester fluorescent whitener				
IT	Polyester fibers				
	RL: USES (Uses) (fluorescent brighteners for, heterocyclic stilbene derivs. as)				
IT	Fluorescent brighteners (heterocyclic stilbene derivs., polyester fibers)				
IT	2362-79-0				
	RL: USES (Uses) (condensation of, with chlorotolylbenzofuran)				
IT	22772-22-1P	22772-23-2P	22772-26-5P	22950-16-9P	25664-50-0P
	25664-53-3P	29335-23-7P	29335-29-3P	29344-58-9P	29347-39-5P
	29347-41-9P	29347-43-1P	29347-55-5P	29347-67-9P	29391-02-4P
	29399-40-4P	51357-97-2P	51357-98-3P	51358-02-2P	51358-03-3P
	51358-05-5P	51358-06-6P	51358-07-7P	51358-09-9P	51358-10-2P
	51358-11-3P	51358-12-4P	51358-13-5P	51358-14-6P	
	RL: IMF (Industrial manufacture); PREP (Preparation) (prepn. of)				
IT	25664-47-5P				
	RL: IMF (Industrial manufacture); PREP (Preparation) (prepn. of, and reaction with benzylideneaniline derivs.)				
IT	51358-01-1				
	RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with benzylideneaniline)				
IT	92-69-3				
	RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with methylphenacyl chloride)				
IT	51358-08-8				
	RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with phenylbenzylideneaniline)				
IT	4209-24-9				
	RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with phenylphenol)				
IT	890-50-6	2362-79-0	18263-29-1	18263-30-4	51357-73-4
	RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with tolylbenzofuran)				
IT	538-51-2	836-41-9			
	RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with tolylbenzofuran derivs.)				
IT	36734-50-6	37564-72-0	51357-99-4	51358-00-0	51358-04-4
	RL: PROC (Process) (treatment of, with polyphosphoric acid)				

REFERENCE 8

AN 80:49271 CA
 TI Fluorescent whiteners
 IN Crounse, Nathan N.; Desai, Kantilal B.
 PA Sterling Drug Inc.

SO Ger. Offen., 28 pp.
 CODEN: GWXXBX
 DT Patent
 LA German
 IC C07D; D06L; C08K
 CC 40-11 (Dyes, Fluorescent Whitening Agents, and Photosensitizers)
 Section cross-reference(s): 37

FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2305970	A1	19730823	DE 1973-2305970	19730207
	US 3833510	A	19740903	US 1972-224296	19720207
	CA 988927	A1	19760511	CA 1973-161971	19730124
	IT 977194	A	19740910	IT 1973-48053	19730205
	GB 1382544	A	19750205	GB 1973-5635	19730205
	JP 48091128	A2	19731127	JP 1973-14851	19730207
PRAI	US 1972-224296		19720207		
AB	Eleven fluorescent whiteners [I; R = H; (RR1) = benzo; R1 = H, Cl, F, CN, Me, MeO, or Ph; R2 = H or Cl; (R2R3) = benzo; R3 = H; R4 = H, Me, or CH2CH2OH; n = 2 or 4; X = O, S], useful for whitening polymer fibers, textiles, and moldings having good light-, bleach-, and heatfastness properties were prep'd. Thus, condensation of 5-chloro-2-(p-tolyl)benzofuran with 4-HO2CC6H4CH:NPh in DMF at 35.deg. in the presence of Me3COK gave fluorescent whitener (I, R = R2 = R3 = R4 = H, R1 = Cl, n = 4, x = O) [50325-20-7], whitening poly(ethylene terephthalate) [25038-59-9] moldings white shades in pinkish-blue region.				
ST	fluorescent whiteners; polyethylene terephthalate brightener; benzofuran carboxystyrylphenyl brightner; styrylphenylbenzofuran brightener; textile brightener; naphthofuran styrylphenyl brightener; synthetic fiber brightener				
IT	Fluorescent brighteners ([(carboxystyryl)phenyl]benzofuran derivs. and analogs, for poly(ethylene terephthalate))				
IT	Poly(oxy-1,2-ethanediylloxycarbonyl-1,4-phenylene carbonyl) RL: USES (Uses) (fluorescent brighteners for, [(carboxystyryl)phenyl]benzofuran derivs. as)				
IT	22772-22-1	22950-16-9			
	RL: USES (Uses)	(condensation of, with anilinophthalide)			
IT	22772-29-8				
	RL: USES (Uses)	(condensation of, with formylbenzoic acid)			
IT	22772-23-2	22772-24-3	22772-26-5	25664-47-5	25664-48-6
	RL: USES (Uses)	(condensation of, with formylbenzoic acids)			
IT	4209-24-9				
	RL: USES (Uses)	(condensation of, with halophenols)			
IT	95-77-2	371-41-5			
	RL: USES (Uses)	(condensation of, with methylphenacyl chloride)			
IT	3939-34-2	33125-69-8			
	RL: USES (Uses)	(condensation of, with tolylbenzofuran derivs. and analogs)			
IT	50325-20-7P	50370-39-3P	50618-24-1P	50618-25-2P	50618-26-3P
	50618-27-4P	50618-28-5P	50618-29-6P	50618-30-9P	50618-31-0P
	50618-32-1P	50618-33-2P	50618-34-3P	50618-35-4P	50618-36-5P
	50618-37-6P	50618-38-7P	50618-39-8P	50618-40-1P	
	RL: IMF (Industrial manufacture); PREP (Preparation)	(prep'n. of)			

AN 71:38699 CA
 TI Anil synthesis. II. Preparation of stilbene and styryl derivatives of
 nitrogen-free oxygen and sulfur heterocycles with aromatic character
 AU Siegrist, Adolf E.; Meyer, Hans R.
 CS Forschungslab. TAP-Abt., CIBA A.-G., Basel, Switz.
 SO Helvetica Chimica Acta (1969), 52(5), 1282-323
 CODEN: HCACAV; ISSN: 0018-019X
 DT Journal
 LA German
 CC 27 (Heterocyclic Compounds (One Hetero Atom))
 AB Ph-substituted furans, benzo[b]furans, naphtho[1,2-b] - and -[2,1-b]furans,
 thiophenes, benzo[b]thiophenes, naphtho[2,1-b]thiophenes, dibenzofurans,
 dibenzothiophenes, phenoxathiins, and thianthrenes, contg. 1 or more Me
 groups in the Ph group and (or) in a benzene ring fused to a heterocycle,
 gave with aromatic aldehyde anils in Me2NCHO, in the presence of KOH or
 tert-BuOK, the corresponding stilbene and styrene derivs.
 ST dibenzothiophenes; dibenzofurans; styrenes heterocyclic; stilbenes
 heterocyclic; benzofurans; benzothiophenes; naphthofurans;
 naphthothiophenes; furans; thiophenes; phenoxathiins; thianthrenes
 IT Dibenzofuran, 3,7-bis(p-phenylstyryl)-, (E,E)-
 Thiophene, 2-[p-(p-methoxystyryl)phenyl]-5-p-tolyl-, (E)-
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 IT 22720-97-4P 22720-98-5P 22720-99-6P 22721-01-3P 22772-22-1P
 22772-23-2P 22772-24-3P 22772-25-4P 22772-26-5P 22772-27-6P
 22772-28-7P 22772-29-8P 22772-30-1P 22772-31-2P 22772-32-3P
 22772-33-4P 22772-34-5P 22772-35-6P 22785-92-8P 22785-93-9P
 22785-94-0P 22785-95-1P 22785-96-2P 22785-97-3P 22785-98-4P
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 22846-69-1P 22846-70-4P 22846-71-5P 22846-72-6P 22861-98-9P
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22862-34-6P 22862-35-7P 22862-36-8P 22862-37-9P 22862-38-0P
22862-39-1P 22862-40-4P 22862-41-5P 22862-42-6P 22862-43-7P
22862-44-8P 22862-78-8P 22950-16-9P 22961-03-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

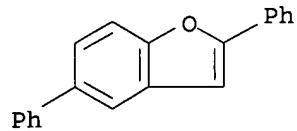
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23013-55-0P 23013-56-1P 23013-57-2P 23013-58-3P 23109-24-2P
25078-51-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 121045-39-4 REGISTRY
 CN Benzofuran, 2,5-diphenyl- (9CI) (CA INDEX NAME)
 OTHER NAMES:
 CN 2,5-Diphenylbenzofuran
 FS 3D CONCORD
 MF C20 H14 O
 SR CA
 LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
 (*File contains numerically searchable property data)

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C6	C6	6	C6	46.150.18	2
C4O-C6	OC4-C6	5-6	C8O	333.200.32	1



Experimental Properties (EPROP)

PROPERTY (CODE)	VALUE	NOTE
Melting Point (MP)	166-168 deg C	(1) IC

(1) Ota, Tomomi; Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) 1988(11) P3029-35 CAPLUS

See HELP PROPERTIES for information about property data sources in REGISTRY.

Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	38410	pH 1	(1) ACD
Bioconc. Factor (BCF)	38410	pH 4	(1) ACD
Bioconc. Factor (BCF)	38410	pH 7	(1) ACD
Bioconc. Factor (BCF)	38410	pH 8	(1) ACD
Bioconc. Factor (BCF)	38410	pH 10	(1) ACD
Boiling Point (BP)	446.8+-14.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	67.79+-3.0 kJ/mol		(1) ACD
Flash Point (FP)	238.7+-12.4 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	2		(1) ACD
H acceptors (HAC)	1		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	66548	pH 1	(1) ACD
Koc (KOC)	66548	pH 4	(1) ACD
Koc (KOC)	66548	pH 7	(1) ACD
Koc (KOC)	66548	pH 8	(1) ACD
Koc (KOC)	66548	pH 10	(1) ACD
logD (LOGD)	6.33	pH 1	(1) ACD
logD (LOGD)	6.33	pH 4	(1) ACD

logD (LOGD)	6.33	pH 7	(1) ACD
logD (LOGD)	6.33	pH 8	(1) ACD
logD (LOGD)	6.33	pH 10	(1) ACD
logP (LOGP)	6.335+/-0.357		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	270.32		(1) ACD
Vapor Pressure (VP)	9.33E-08 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.76 ((C) 1994-2003 ACD)

4 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 138:153392 CA
 TI Synthesis of 2-Arylbenzo[b]furans via Copper(I)-Catalyzed Coupling of o-Iodophenols and Aryl Acetylenes
 AU Bates, Craig G.; Saejueng, Pranorm; Murphy, Jaclyn M.; Venkataraman, D.
 CS Department of Chemistry, University of Massachusetts-Amherst, Amherst, MA, 01003, USA
 SO Organic Letters (2002), 4(26), 4727-4729
 CODEN: ORLEF7; ISSN: 1523-7060
 PB American Chemical Society
 DT Journal
 LA English
 CC 27-7 (Heterocyclic Compounds (One Hetero Atom))
 AB We report a copper(I)-catalyzed procedure for the synthesis of 2-arylbenzo[b]furans. This protocol can be used to synthesize a variety of 2-arylbenzo[b]furans in good to excellent yields. This method can tolerate a variety of functional groups, does not require the use of expensive additives, and is palladium-free.
 ST copper coupling iodophenol arylacetylene; benzofuran aryl prepn
 IT Coupling reaction
 Coupling reaction catalysts
 (2-arylbenzo[b]furans via copper(I)-catalyzed coupling of o-iodophenols and arylacetylenes)
 IT 15709-74-7P
 RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (2-arylbenzo[b]furans via copper(I)-catalyzed coupling of o-iodophenols and arylacetylenes)
 IT 25753-81-5P 25753-84-8P 33989-10-5P 391684-10-9P
 RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
 (2-arylbenzo[b]furans via copper(I)-catalyzed coupling of o-iodophenols and arylacetylenes)
 IT 66-71-7, 1,10-Phenanthroline 106-44-5, 4-Methylphenol, reactions
 366-18-7, 2,2'-Bipyridine 484-11-7, Neocuproine 533-58-4, 2-Iodophenol
 536-74-3, Ethynylbenzene 603-35-0, Triphenylphosphine, reactions
 766-97-2, p-Tolylacetylene 767-00-0, 4-Cyanophenol 767-91-9,
 o-Anisylacetylene 768-60-5, p-Anisylacetylene 2296-23-3,
 3-Iodo-4-hydroxybenzonitrile 2499-64-1, p-Ethynylstyrene 3032-92-6,
 4-Ethynylbenzonitrile 3034-86-4, Methyl 4-ethynylbenzoate 7789-45-9,
 Cupric bromide 16188-57-1, 2-Iodo-4-methylphenol 19004-19-4
 33577-99-0, Methyl 2-ethynylbenzoate 38941-98-9,
 4-tert-Butyl-2-iodophenol 42472-69-5, 4'-Ethynylacetophenone 71031-48-6,
 3-Iodo-4-biphenylol 71643-66-8, 4-Chloro-2-iodophenol 207115-22-8,
 4-Bromo-2-iodophenol

RL: RCT (Reactant); RACT (Reactant or reagent)
 (2-arylbenzo[b]furans via copper(I)-catalyzed coupling of o-iodophenols
 and arylacetylenes)

IT 106678-35-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (2-arylbenzo[b]furans via copper(I)-catalyzed coupling of o-iodophenols
 and arylacetylenes)

IT 1839-72-1P, 2-Phenylbenzofuran 13141-26-9P 18761-36-9P 19234-04-9P
 25664-48-6P, 2-p-Tolylbenzofuran 25871-52-7P 36078-99-6P 41013-94-9P
 42926-53-4P 69976-43-8P 79008-77-8P 121045-39-4P 122778-95-4P
 132932-61-7P 247136-48-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (2-arylbenzo[b]furans via copper(I)-catalyzed coupling of o-iodophenols
 and arylacetylenes)

RE.CNT 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD

- (1) Arcadi, A; J Org Chem 1996, V61, P9280 CAPLUS
- (2) Arcadi, A; Synlett 1999, P1432 CAPLUS
- (3) Arcadi, A; Synthesis 1986, P749 CAPLUS
- (4) Bates, C; Org Lett 2002, V4, P2803 CAPLUS
- (5) Cacchi, S; Tetrahedron Lett 1998, V39, P5101 CAPLUS
- (6) Castro, C; J Org Chem 1966, V31, P4071 CAPLUS
- (7) Doad, G; Tetrahedron Lett 1989, V30, P1597 CAPLUS
- (8) Donnelly, D; Comprehensive Heterocyclic Chemistry 1984, V4
- (9) Dyker, G; J Org Chem 1993, V58, P6426 CAPLUS
- (10) Erber, S; Anti-Cancer Drug Des 1991, V6, P417 CAPLUS
- (11) Fagan, P; J Am Chem Soc 2000, V122, P5043 CAPLUS
- (12) Fancelli, D; Tetrahedron Lett 1997, V38, P2311 CAPLUS
- (13) Goodbrand, H; J Org Chem 1999, V64, P670 CAPLUS
- (14) Gujadhur, R; Org Lett 2001, V3, P4315 CAPLUS
- (15) Gujadhur, R; Synth Commun 2001, V31, P2865 CAPLUS
- (16) Gujadhur, R; Tetrahedron Lett 2001, V42, P4791 CAPLUS
- (17) Hennessy, E; Org Lett 2002, V4, P269 CAPLUS
- (18) Kabalka, G; Tetrahedron 2001, V57, P8017 CAPLUS
- (19) Kalinin, A; J Org Chem 1999, V64, P2986 CAPLUS
- (20) Katritzky, A; J Org Chem 2001, V66, P5613 CAPLUS
- (21) Kiyomori, A; Tetrahedron Lett 1999, V40, P2657 CAPLUS
- (22) Klapars, A; J Am Chem Soc 2001, V123, P7727 CAPLUS
- (23) Kundu, N; J Chem Soc, Perkin Trans 1 1997, P2815 CAPLUS
- (24) Kwong, F; Org Lett 2002, V4, P581 CAPLUS
- (25) Larock, R; J Org Chem 1995, V60, P3270 CAPLUS
- (26) Ma, D; J Am Chem Soc 1998, V120, P12459 CAPLUS
- (27) Malamas, M; J Med Chem 2000, V43, P1293 CAPLUS
- (28) Marcoux, J; J Am Chem Soc 1997, V119, P10539 CAPLUS
- (29) McAllister, G; J Chem Soc, Perkin Trans 1 1998, P3453 CAPLUS
- (30) McCallion, G; Curr Org Chem 1999, V3, P67 CAPLUS
- (31) Nan, Y; Org Lett 2000, V2, P297 CAPLUS
- (32) Torii, S; Synlett 1992, P515 CAPLUS
- (33) Watanabe, Y; J Heterocycl Chem 1993, V30, P445 CAPLUS
- (34) Wolter, M; Org Lett 2001, V3, P3803 CAPLUS
- (35) Wolter, M; Org Lett 2002, V4, P973 CAPLUS
- (36) Zhang, S; J Org Chem 1997, V62, P2312 CAPLUS

REFERENCE 2

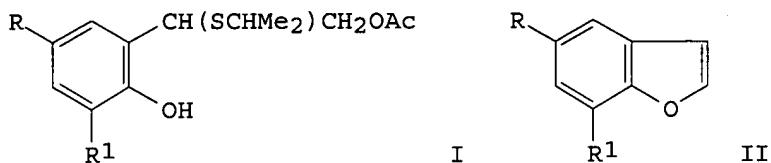
AN 118:244399 CA
 TI Study on the mechanism of photofading of magenta azomethine dye. Part (I).
 Reaction with active oxygen
 AU Yang, Xiaonan; Shi, Junying
 CS Res. Inst. Spec. Chem., East China Univ. Chem. Technol., Shanghai, 200237,
 Peop. Rep. China
 SO Gaodeng Xuexiao Huaxue Xuebao (1993), 14(2), 204-8
 CODEN: KTHPDM; ISSN: 0251-0790
 DT Journal

LA Chinese
CC 74-2 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
AB The photofading of magenta azomethine dye (MAD) was studied by HPLC, UV-visible spectra. MAD was not a sensitizer but a good acceptor of active O species. The phys. and chem. quenching rate const. of MAD with active O was measured by HPLC. Phys. quenching was the main pathway in the quenching process. Singlet O (1O2) played a dominant role in the photofading of MAD sensitized by Methylene Blue or Rose Bengal.
ST photofading magenta azomethine dye oxygen acceptor
IT Oxidation, photochemical
 (of magenta azomethine dye by singlet oxygen and superoxide anion)
IT Photography, color
 (photofading of magenta azomethine dye in reactions with active oxygen species in relation to)
IT 7506-92-5P
 RL: FORM (Formation, nonpreparative); PREP (Preparation)
 (formation of, in reaction of epinephrine with superoxide radical, photofading of magenta azomethine dye in relation to)
IT 61-73-4, Methylene blue 11121-48-5, Rose Bengal
 RL: USES (Uses)
 (photofading of magenta azomethine dye sensitized by, reactions with singlet oxygen and superoxygen anion in)
IT 121045-39-4
 RL: USES (Uses)
 (photooxidn. of magenta dye by singlet oxygen and superoxide anion in system contg.)
IT 51-43-4
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with superoxide ion, photofading of magenta azomethine dye in relation to)
IT 7782-44-7, Oxygen, reactions 11062-77-4, Superoxide
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (singlet, reactions of, in photofading of magenta azomethine dye)

REFERENCE 3

AN 117:25738 CA
TI Singlet oxygen chemistry. VI. Kinetics of photooxygenation of 2,5-diphenylbenzofuran (DPBF) induced by hypocreallin A (HA) in micelles
AU Jiang, Xianfeng; Wang, Duoyuan
CS Inst. Photogr. Chem., Acad. Sin., Beijing, 100101, Peop. Rep. China
SO Huaxue Xuebao (1992), 50(4), 391-6
CODEN: HHHPA4; ISSN: 0567-7351
DT Journal
LA Chinese
CC 22-7 (Physical Organic Chemistry)
AB The kinetics of photooxygenation of DPBF induced by HA in a micellar aq. medium were investigated.
ST photooxidn diphenylbenzofuran hypocreallin A; benzofuran diphenyl photooxidn kinetics
IT Micelles
 (effect of, on kinetics of photooxidn. of diphenylbenzofuran induced by hypocreallin A)
IT Kinetics of oxidation
 (photochem., of diphenylbenzofuran induced by hypocreallin A in micelles)
IT 123940-54-5
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (photooxygenation of diphenylbenzofuran induced by, in micelles)
IT 121045-39-4, 2,5-Diphenylbenzofuran
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (photooxygenation of, induced by hypocreallin A in micelles)

AN 111:7155 CA
TI Selective preparation and cyclization of 2-(2-hydroxyphenyl)-2-(isopropylthio)ethanols. New Synthesis of 1-benzofurans
AU Ota, Tomomi; Hasegawa, Shun; Inoue, Seiichi; Sato, Kikumasa
CS Fac. Eng., Yokohama Natl. Univ., Yokohama, 240, Japan
SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1988), (11), 3029-35
CODEN: JCPRB4; ISSN: 0300-922X
DT Journal
LA English
CC 27-6 (Heterocyclic Compounds (One Hetero Atom))
GI



AB	Reaction of 2,4-R(R1)C6H3OH (R = H, R1 = H, Ph, Me, MeO, Cl, cyclohexyl, etc.; R = Me, MeO, Cl, R1 = H) with Me2CHSCH2CH2OMe activated by SO2Cl2 afforded 2-[2-acetoxy-1-(isopropylthio)ethyl]phenols I (R, R1 = as above) regioselectively, via [2,3]sigmatropic rearrangement of phenoxy sulfonium ylides. The ortho-alkylated phenols thus obtained were cyclized with conc. HCl in MeOCH2CH2OH to 1-benzofuran II (R, R1 = as above). 2-Methyl- and 2-phenyl-1-benzofuran were prep'd. similarly.
ST	benzofuran; acetoxyisopropylthioethylphenol regioselective prep'n cyclization; phenol alkylation isopropylthioethyl acetate
IT	Alkylation (of phenols with isopropylthio acetates and sulfonyl chloride, in synthesis of benzofurans)
IT	Cyclocondensation reaction (intramol., of (hydroxyphenyl)(isopropylthio)ethanols, benzofurans from)
IT	5862-49-7 RL: RCT (Reactant); RACT (Reactant or reagent) (alkylation by, of phenols in presence of sulfonyl chloride)
IT	75-33-2, 2-Propanethiol RL: RCT (Reactant); RACT (Reactant or reagent) (alkylation of, with chloropropanol and phenacyl chloride)
IT	90-05-1, 2-Methoxyphenol 92-69-3, 4-Phenylphenol 95-48-7, 2-Cresol, reactions 95-57-8, 2-Chlorophenol 100-02-7, 4-Nitrophenol, reactions 106-44-5, 4-Cresol, reactions 106-48-9, 4-Chlorophenol 108-95-2, Phenol, reactions 120-47-8, Ethyl 4-hydroxybenzoate 150-76-5, 4-Methoxyphenol 1131-60-8, 4-Cyclohexylphenol RL: RCT (Reactant); RACT (Reactant or reagent) (alkylation of, with isopropylthioethyl acetates and sulfonyl chloride)
IT	122-94-1, 4-Butoxyphenol RL: RCT (Reactant); RACT (Reactant or reagent) (alkylation of, with isopropylthiomethyl ethyl acetate)
IT	99-93-4, p-Hydroxyacetophenone 105-67-9, 2,4-Dimethylphenol 123-08-0, 4-Hydroxybenzaldehyde RL: RCT (Reactant); RACT (Reactant or reagent) (alkylation of, with isopropylthiophenylethyl acetate)
IT	127-00-4, 1-Chloropropan-2-ol 532-27-4, Phenacyl chloride RL: RCT (Reactant); RACT (Reactant or reagent) (alkylation of, with propanethiol)
IT	121045-44-1

RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of)

IT 64955-36-8P, 1-(Isopropylthio)propan-2-ol 121045-46-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and acetylation of)

IT 64955-39-1P 121045-17-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and alkylation by, of phenols in presence of sulfonyl chloride)

IT 66502-11-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and borohydride redn. of)

IT 111437-45-7P 121045-14-5P 121045-18-9P 121045-20-3P 121045-21-4P
121045-22-5P 121045-23-6P 121045-24-7P 121045-27-0P 121045-28-1P
121045-29-2P 121045-30-5P 121045-31-6P 121045-32-7P 121045-33-8P
121045-34-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and intramol. cyclocondensation of, benzofuran from)

IT 271-89-6P, Benzofuran 1839-72-1P, 2-Phenylbenzofuran 4265-25-2P,
2-Methylbenzofuran 7168-85-6P, 7-Methoxybenzofuran 7182-32-3P,
5-Methoxy-2-phenylbenzofuran 13391-27-0P 13391-28-1P,
5-Methoxybenzofuran 14385-51-4P, 7-Methoxy-2-phenylbenzofuran 17059-52
-8P, 7-Methylbenzofuran 18441-43-5P, 5-Methylbenzofuran 18761-31-4P,
5-Nitrobenzofuran 23145-05-3P, 5-Chlorobenzofuran 24410-55-7P
25871-52-7P 29040-46-8P, 2,5-Dimethylbenzofuran 35664-71-2P
42180-82-5P, 5-Chloro-2-methylbenzofuran 50543-55-0P 59020-74-5P
59483-17-9P, 5,7-Dimethyl-2-phenylbenzofuran 121045-15-6P 121045-16-7P
121045-19-0P 121045-35-0P 121045-36-1P 121045-37-2P 121045-38-3P
121045-39-4P 121045-40-7P 121045-41-8P 121045-42-9P 121045-43-0P
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121045-51-0P 121045-52-1P 121045-53-2P 121045-54-3P 121045-55-4P
121836-00-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

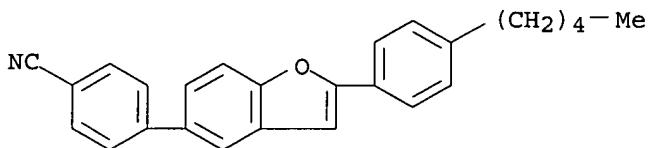
IT 121045-26-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn., dehydrogenation, and transesterification of)

IT 121045-25-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn., transesterification and intramol. cyclocondensation of)

RN 331834-02-7 REGISTRY
 CN Benzonitrile, 4-[2-(4-pentylphenyl)-5-benzofuranyl]- (9CI) (CA INDEX
 NAME)
 FS 3D CONCORD
 MF C26 H23 N O
 SR CA
 LC STN Files: CA, CAPLUS

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C6	C6	6	C6	46.150.18	2
C4O-C6	OC4-C6	5-6	C8O	333.200.32	1



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1090652	pH 1	(1) ACD
Bioconc. Factor (BCF)	1090652	pH 4	(1) ACD
Bioconc. Factor (BCF)	1090652	pH 7	(1) ACD
Bioconc. Factor (BCF)	1090652	pH 8	(1) ACD
Bioconc. Factor (BCF)	1090652	pH 10	(1) ACD
Boiling Point (BP)	548.0 +/- 35.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	82.75 +/- 3.0 kJ/mol		(1) ACD
Flash Point (FP)	285.2 +/- 46.7 deg C		(1) ACD
H acceptors (HAC)	2		(1) ACD
H donors (HD)	0		(1) ACD
Koc (KOC)	730036	pH 1	(1) ACD
Koc (KOC)	730036	pH 4	(1) ACD
Koc (KOC)	730036	pH 7	(1) ACD
Koc (KOC)	730036	pH 8	(1) ACD
Koc (KOC)	730036	pH 10	(1) ACD
logD (LOGD)	8.25	pH 1	(1) ACD
logD (LOGD)	8.25	pH 4	(1) ACD
logD (LOGD)	8.25	pH 7	(1) ACD
logD (LOGD)	8.25	pH 8	(1) ACD
logD (LOGD)	8.25	pH 10	(1) ACD
logP (LOGP)	8.247 +/- 0.412		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	365.47		(1) ACD
Vapor Pressure (VP)	4.62E-12 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris

2 REFERENCES IN FILE CA (1907 TO DATE)
 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 136:142912 CA
 TI The synthesis and transition temperatures of 2-(4-alkyl- and 4-alkoxy-phenyl)-5-cyano-1-benzofurans and related diaryl-1-benzofurans - an assessment of how deviations from linearity and conformational effects in a core unit affect mesogenicity
 AU Friedman, Mark R.; Toyne, Kenneth J.; Goodby, John W.; Hird, Michael
 CS Liquid Crystals and Advanced Organic Materials Research Group, The Department of Chemistry, The University of Hull, Hull, HU6 7RX, UK
 SO Journal of Materials Chemistry (2001), 11(11), 2759-2772
 CODEN: JMACEP; ISSN: 0959-9428
 PB Royal Society of Chemistry
 DT Journal
 LA English
 CC 75-11 (Crystallography and Liquid Crystals)
 Section cross-reference(s): 27
 AB The synthesis and transition temps. are reported for several 2-(4-alkyl- and 4-alkoxy-phenyl)-5-cyano-1-benzofurans, 2-(4'-alkylbiphenyl-4-yl)-5-cyano- and 5-(4'-alkylbiphenyl-4-yl)-2-cyano-1-benzofurans, and for compds. with other combinations of terminal alkyl and cyano groups in 2,5-disubstituted-1-benzofurans contg. two Ph units; some isolated examples of related cyclohexane systems are also presented. The mesogenic behavior of these compds. and several intermediates (e.g. amides, acids and esters) is discussed and the transition temps. are rationalized on the following basis (a) 1-benzofuran is a superior core unit to benzene, (b) 2,5-disubstitution in 1-benzofuran gives a bent core which adversely affects mesogenicity, to an extent which depends on its position in the core, (c) antiparallel assocns. in terminal cyano compds. can eliminate the disadvantage of a bent core structure, and (d) 2-aryl-1-benzofurans have negligible inter-annular twist but 5-aryl-1-benzofurans have similar inter-annular twist to that in biphenyls.
 ST liq crystal alkoxyphenylcyanobenzofuran alkylphenylcyanobenzofuran prepn property; benzofuran cyano deriv liq crystal prepn property
 IT Liquid crystals
 (prepn. and properties of (alkyl- and alkoxyphenyl)cyanobenzofurans and related diarylbenzofurans)
 IT Liquid crystals
 (transitions; of (alkyl- and alkoxyphenyl)cyanobenzofurans and related diarylbenzofurans)
 IT 331833-92-2
 RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)
 (liq. crystal properties of)
 IT 79002-39-4P, 5-Benzofurancarbonitrile 331834-10-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. and conversion to boronic acid)
 IT 118780-12-4P 393184-37-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. and cyclization of)
 IT 331833-89-7P 331834-15-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. and dehydration of)
 IT 331833-88-6P 331834-14-1P
 RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); PROC (Process); RACT (Reactant or reagent)
(prepn. and liq. crystal properties and amidation of)

IT 247121-10-4P
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP
(Physical process); RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); PROC (Process); RACT (Reactant or reagent)
(prepn. and liq. crystal properties and carboxylation of)

IT 331833-86-4P 331833-91-1P
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP
(Physical process); RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); PROC (Process); RACT (Reactant or reagent)
(prepn. and liq. crystal properties and hydrolysis of)

IT 331833-82-0P 331833-85-3P 331833-90-0P 331833-94-4P 331833-96-6P
331833-98-8P 331834-02-7P 331834-05-0P 331834-09-4P 331834-12-9P
331834-16-3P 331834-17-4P
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP
(Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC
(Process)
(prepn. and liq. crystal properties of)

IT 156480-87-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and reaction with benzofuranboronic acid)

IT 85017-60-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and reaction with bromobenzofuranboronic acid)

IT 4923-87-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and reaction with heptylphenylboronic acid)

IT 331833-99-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and reaction with iodopentylbenzene)

IT 53020-42-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and reaction with pentylbenzoic acid)

IT 38573-37-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and reaction with triphenylphosphine)

IT 331833-79-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and reactions of)

IT 393184-38-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and reactions with heptylbenzoic acid and nonyloxybenzoic acid)

IT 331833-83-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and reactions with propylphenyl bromide, pentylphenyl bromide
and pentylbiphenyl bromide)

IT 331833-84-2P 331834-21-0P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and thermal behavior of)

RE.CNT 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD

- (1) Angeloni, A; Ann Chim (Rome) 1963, V53, P1665 CAPLUS
- (2) Benassi, R; J Chem Soc, Perkin Trans 2 1987, P1443 CAPLUS
- (3) Brownsey, G; J Phys Lett 1981, V42, P135 CAPLUS
- (4) Castellano, J; J Org Chem 1968, V33, P3501 CAPLUS

- (5) Coulson, D; Inorg Synth 1972, V13, P121
 (6) Demus, D; Flussige Kristalle in Tabellen 1974, VI
 (7) Demus, D; Flussige Kristalle in Tabellen 1984, VII
 (8) Deutscher, H; Z Chem 1977, V17, P64 CAPLUS
 (9) Dunmur, D; Liq Cryst 1986, V1, P169 CAPLUS
 (10) Friedman, M; Liq Cryst 2001, V28, P901 CAPLUS
 (11) Goto, Y; JP 85125489 1985
 (12) Gray, G; J Chem Soc, Perkin Trans 2 1989, P2041 CAPLUS
 (13) Gray, G; Mol Cryst Liq Cryst 1991, V195, P221 CAPLUS
 (14) Gray, G; Mol Cryst Liq Cryst 1991, V204, P91 CAPLUS
 (15) Haase, W; Mol Cryst Liq Cryst 1983, V97, P131 CAPLUS
 (16) Hercouet, A; Tetrahedron 1981, V37, P2867 CAPLUS
 (17) Hird, M; Liq Cryst 1993, V15, P123 CAPLUS
 (18) Hird, M; Mol Cryst Liq Cryst 1998, V323, P1 CAPLUS
 (19) Karamysheva, L; Liq Cryst 1991, V10, P875 CAPLUS
 (20) Kasztreiner, E; DE 2137538 1972 CAPLUS
 (21) Kaszynski, P; Mol Cryst Liq Cryst 1995, V260, P315 CAPLUS
 (22) Kurdukar, R; Proc Indian Acad Sci, Sect A 1963, V58, P336 CAPLUS
 (23) LaPlanche, L; J Phys Chem 1965, V69, P1482 CAPLUS
 (24) Leadbetter, A; J Phys C Solid State Phys 1975, V36, P37
 (25) Rabindran, K; Proc Indian Acad Sci Sect A 1952, V36, P405
 (26) Rappe, A; J Am Chem Soc 1992, V114, P10024 CAPLUS
 (27) Rene, L; Bull Soc Chim Fr 1974, P475 CAPLUS
 (28) Schad, H; J Chem Phys 1981, V75, P880 CAPLUS
 (29) Schad, H; J Chem Phys 1983, V79, P5710 CAPLUS
 (30) Schad, H; J Chem Phys 1984, V81, P1514 CAPLUS
 (31) Spagnolo, P; J Chem Soc, Perkin Trans 1 1972, P556 CAPLUS
 (32) Tilak, B; Tetrahedron 1960, V9, P76 CAPLUS
 (33) Vill, V; Liquid Crystal Database of liquid crystalline compounds for Personal Computers 1999, V3, PD-20259

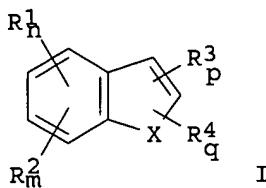
REFERENCE 2

AN 134:273622 CA
 TI Liquid crystal compounds
 IN Goodby, John William; Toyne, Kenneth Johnson; Hird, Michael; Friedman, Mark Richard; Jones, John Clifford
 PA Secretary of State for Defence, UK
 SO PCT Int. Appl., 140 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 IC ICM C07D307-78
 ICS C07D333-52; C09K019-34
 CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
 Section cross-reference(s): 27, 75

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001021606	A1	20010329	WO 2000-GB3545	20000915
	W: GB, JP, US				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	EP 1214306	A1	20020619	EP 2000-962671	20000915
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY				
	JP 2003509507	T2	20030311	JP 2001-524985	20000915
PRAI	GB 1999-22179	19990921			
	GB 2000-9267	20000417			
	WO 2000-GB3545		20000915		

GI



- AB The invention relates to novel compds. having a fused heterocyclic ring that have properties of liq. crystals, together with processes for their prepn. and liq. crystal devices incorporating them. A liq. crystal compd. (I) where X is O, S or Se, and R1, R2, R3, R4, m, n, p and q are as specified in the application. Liq. crystal devices comprising the compds. are also claimed.
- ST liq crystal display device heterocyclic ring benzofuran benzothiophene
- IT Liquid crystal displays
Liquid crystals
(prepn. of benzofuran derivs. and their use as liq. crystal compds. in display devices)
- IT Heterocyclic compounds
RL: NUU (Other use, unclassified); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(prepn. of benzofuran derivs. and their use as liq. crystal compds. in display devices)
- IT 588-93-2P, 1-Bromo-4-propylbenzene 1987-50-4P, 4-Heptylphenol 4923-87-9P, 5-Bromobenzo[b]thiophene 6418-38-8P, 2,3-Difluorophenol 10242-08-7P 10242-11-2P 19514-91-1P, 4,6-Diodoresorcinol 23145-07-5P, 5-Bromobenzo[b]furan 23703-22-2P, 1-Bromo-4-hexylbenzene 35351-21-4P 35351-22-5P 35351-45-2P 35351-47-4P 38573-37-4P 50551-56-9P 51554-93-9P, 1-Bromo-4-octylbenzene 51554-94-0P 51554-95-1P, 1-Bromo-4-pentylbenzene 53020-42-1P 57774-34-2P, 4-Cyano-4'-iodobiphenyl 63619-59-0P 76287-49-5P, 1-Bromo-4-heptylbenzene 79002-39-4P, 5-Cyanobenzo[b]furan 79887-19-7P, 4-Octyloxyphenylacetylene 84102-69-2P, Ethyl 5-bromobenzo[b]furan-2-carboxylate 85017-60-3P 96693-05-9P, 1-Bromo-4-octyloxybenzene 105365-50-2P 118780-12-4P 121219-12-3P 121219-16-7P 121554-18-5P 125151-57-7P 126334-32-5P, 1-(2,3-Difluorophenyl)-1-heptanol 126334-34-7P, 1,2-Difluoro-3-heptylbenzene 126334-37-0P 126747-14-6P 129969-69-3P, 2-(4-Bromophenoxy)acetaldehyde dimethyl acetal 131894-91-2P, 1-Heptyl-4-iodobenzene 133997-05-4P 134150-01-9P, 4-Propylbenzeneboronic acid 156480-87-4P 163129-11-1P 173392-87-5P 247121-10-4P 256383-44-5P 256383-45-6P 331833-66-0P 331833-67-1P 331833-68-2P 331833-75-1P 331833-76-2P 331833-77-3P 331833-78-4P 331833-79-5P 331833-80-8P 331833-81-9P 331833-83-1P 331833-87-5P 331833-95-5P 331833-98-8P 331833-99-9P 331834-00-5P 331834-03-8P 331834-04-9P 331834-06-1P 331834-07-2P 331834-08-3P 331834-10-7P 331834-11-8P 331834-13-0P 331834-15-2P 331834-18-5P 331834-35-6P 331834-36-7P 331834-41-4P 331834-42-5P 331834-43-6P 331834-45-8P 331834-47-0P, 5-(1-Heptynyl-4-phenyl)benzo[b]furan 331834-48-1P, 5-(1-Heptynyl-4-phenyl)benzo[b]furan-2-boronic acid 331834-51-6P 331834-52-7P 331834-54-9P 331834-55-0P 331834-57-2P 331834-58-3P 331834-59-4P 331834-60-7P 331834-62-9P 331834-64-1P 331834-65-2P 331834-67-4P 331834-68-5P 331834-69-6P 331834-70-9P 331834-72-1P 331942-28-0P
RL: DEV (Device component use); NUU (Other use, unclassified); RCT (Reactant); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of benzofuran derivs. and their use as liq. crystal compds. in display devices)
- IT 331833-69-3P 331833-70-6P 331833-71-7P 331833-72-8P 331833-73-9P
331833-74-0P 331833-82-0P 331833-84-2P 331833-85-3P 331833-86-4P
331833-88-6P 331833-89-7P 331833-90-0P 331833-91-1P 331833-92-2P

331833-93-3P 331833-94-4P 331833-96-6P 331833-97-7P 331834-02-7P
331834-05-0P 331834-09-4P 331834-12-9P 331834-14-1P 331834-16-3P
331834-17-4P 331834-19-6P 331834-20-9P 331834-21-0P 331834-22-1P
331834-23-2P 331834-24-3P 331834-25-4P 331834-26-5P 331834-27-6P
331834-28-7P 331834-29-8P 331834-30-1P 331834-31-2P 331834-32-3P
331834-33-4P 331834-34-5P 331834-37-8P 331834-38-9P 331834-39-0P
331834-40-3P 331834-44-7P 331834-46-9P, 2- (4-Heptylphenyl)-5- (1-
heptynyl-4-phenyl)benzo[b]furan 331834-50-5P 331834-53-8P
331834-56-1P 331834-61-8P 331834-63-0P 331834-66-3P 331834-71-0P
331834-73-2P 331837-34-4P

RL: DEV (Device component use); NUU (Other use, unclassified); SPN
(Synthetic preparation); TEM (Technical or engineered material use); PREP
(Preparation); USES (Uses)
(prepn. of benzofuran derivs. and their use as liq. crystal compds. in
display devices)

RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD

- (1) Basf Ag; DE 19630068 A 1998 CAPLUS
- (2) Canon Kk; EP 0666262 A 1995 CAPLUS
- (3) Canon Kk; EP 0678509 A 1995 CAPLUS
- (4) Canon Kk; JP 07179856 A 1995 CAPLUS
- (5) Merck Patent GmbH; DE 19900517 A 1999 CAPLUS
- (6) Merck Patent GmbH; DE 19909760 A 1999 CAPLUS
- (7) Merck Patent GmbH; DE 19909761 A 1999 CAPLUS
- (8) Shtarev; J ORG CHEM 1997, V62(16), P5608 CAPLUS

AN 1976:123420 CAPLUS
 DN 84:123420
 TI Sulfo group-containing heterocycles
 IN Meyer, Hans Rudolf
 PA Ciba-Geigy A.-G., Switz.
 SO Ger. Offen., 65 pp.
 CODEN: GWXXBX
 DT Patent
 LA German
 IC C07D; D06L
 CC 40-11 (Dyes, Fluorescent Whitening Agents, and Photosensitizers)
 FAN.CNT 8

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2525683	A1	19760102	DE 1975-2525683	19750609
	CH 592704	A	19771115	CH 1974-8033	19740612
	US 4013642	A	19770322	US 1975-585739	19750610
	JP 51011979	A2	19760130	JP 1975-71422	19750612
	US 4177347	A	19791204	US 1978-908600	19780523
	US 4276188	A	19810630	US 1979-62822	19790801
PRAI	CH 1974-8031		19740612		
	CH 1974-8033		19740612		
	CH 1974-8032		19740612		
	CH 1974-8038		19740612		
	US 1975-585540		19750610		
	US 1975-585542		19750610		
	US 1976-749193		19761209		
	US 1976-749643		19761210		
	US 1977-860819		19771215		

GI For diagram(s), see printed CA Issue.
 AB Fluorescent whiteners (I, R = H, SO₃M, C₆H₄SO₃M; M = Na, K, amine; n = 0, 1) were prep'd. and whitened cotton and polyamide fibers and polyacrylonitrile [25014-41-9] films. Thus, KOCMe₃ was added to a soln. of 2-p-tolylbenzofuran [25664-48-6] and 2-NaO₃SC₆H₄CH:NPh [40567-08-6] in DMF, the soln. held at room temp. for 0.5 hr by external cooling, heated at 60.degree. for 0.5 hr, heated at 80.degree. for 1 hr, cooled, and H₂O added to give the Na-K salt of I(R = 2-SO₃M, n = 1, M = H) [58566-39-5].
 ST polyacrylonitrile fluorescent brightener; benzofuran fluorescent brightener; sulfo group fluorescent brightener; cotton fluorescent brightener; polyamide fiber fluorescent brightener; stilbene fluorescent brightener
 IT Polyester fibers
 RL: USES (Uses)
 (fluorescent brighteners for, sulfostyrylbenzofuran derivs.)
 IT Fluorescent brighteners
 (sulfostyrylbenzofuran derivs., cotton and polyamide fibers and polyacrylonitrile)
 IT Benzenesulfonic acid, 2-[2-[4-(2-benzofuranyl)phenyl]ethenyl]-, potassium-sodium salt
 RL: IMF (Industrial manufacture); PREP (Preparation)
 (fluorescent brightener, for cotton and polyamide fibers, prep'n. of)
 IT 58566-25-9 58566-26-0 58566-29-3
 RL: USES (Uses)
 (fluorescent brightener, for cotton and polyamide fibers; prep'n. of)
 IT 25014-41-9
 RL: USES (Uses)
 (fluorescent brighteners for, styrylbenzofuran derivs. as)
 IT 25014-41-9
 RL: USES (Uses)
 (fluorescent brighteners for, sulfostyrylbenzofuran derivs.)
 IT 58566-27-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prep'n. and reaction with DMF)

IT 40567-08-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. and reaction with tolylbenzofuran)

IT 20143-56-0P 54923-55-6P 58331-41-2P 58419-38-8P 58566-30-6P
 58566-31-7P 58566-32-8P 58566-33-9P 58566-34-0P 58566-35-1P
 58566-36-2P 58566-37-3P **58566-38-4P**
 RL: IMF (Industrial manufacture); PREP (Preparation)
 (prepn. of)

IT 13736-22-6 58331-45-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with aniline)

IT 1008-72-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with chloroaniline)

IT 106-47-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with sodium formylbenzenesulfonate)

IT 25664-48-6 58566-30-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with sodium formylbenzenesulfonate anil)

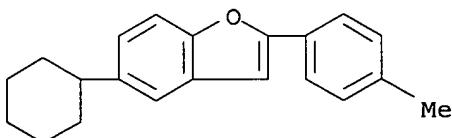
IT 58370-54-0 58419-46-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with tolylbenzofuran)

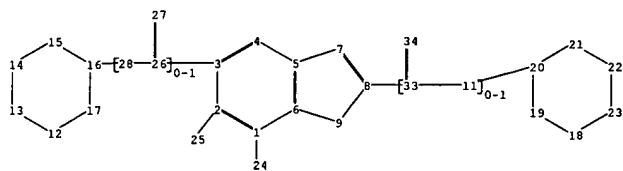
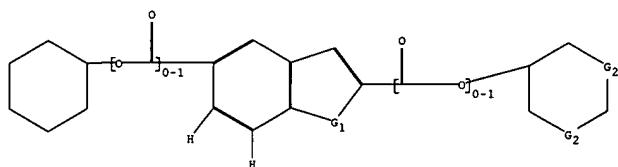
IT 3218-36-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (sulfonation of)

IT 62-53-3, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (with sodium formylbenzenesulfonate)

IT **58566-38-4P**
 RL: IMF (Industrial manufacture); PREP (Preparation)
 (prepn. of)

RN 58566-38-4 CAPLUS
 CN Benzofuran, 5-cyclohexyl-2-(4-methylphenyl)- (9CI) (CA INDEX NAME)





chain nodes :
 11 24 25 26 27 28 33 34

ring nodes :

1 2 3 4 5 6 7 8 9 12 13 14 15 16 17 18 19 20 21 22 23

chain bonds :

1-24 2-25 3-26 8-33 11-20 11-33 16-28 26-27 26-28 33-34

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 12-13 12-17 13-14 14-15 15-16
 16-17 18-19 18-23 19-20 20-21 21-22 22-23

exact/norm bonds :

1-24 2-25 3-26 5-7 6-9 7-8 8-9 8-33 11-20 11-33 12-13 12-17 13-14 14-15
 15-16 16-17 16-28 18-19 18-23 19-20 20-21 21-22 22-23 26-27 26-28 33-34

normalized bonds :

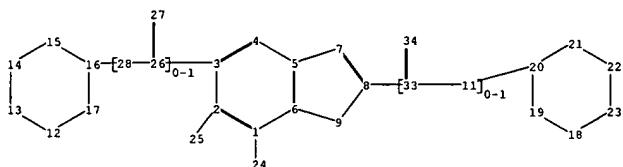
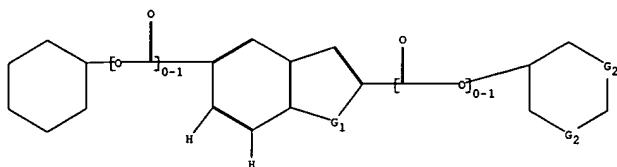
1-2 1-6 2-3 3-4 4-5 5-6

G1:O,S

G2:C,O,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 11:CLASS 12:Atom
 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom
 23:Atom 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 33:Atom 34:CLASS



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ring nodes :

1 2 3 4 5 6 7 8 9 12 13 14 15 16 17 18 19 20 21 22 23
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normalized bonds :

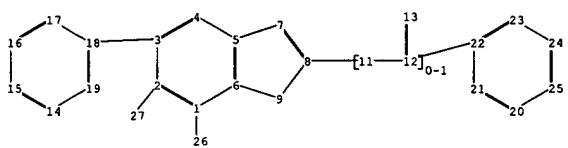
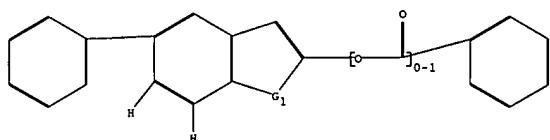
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13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom
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chain nodes :
 11 12 13 26 27

ring nodes :

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chain bonds :

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 12:CLASS 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:CLASS 27:CLASS